THE VIBRATIONALLY DRIVEN H-ATOM ABSTRACTION FROM METHANE BY BROMINE RADICALS

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In an effort to understand how the Polanyi rules can be extended from radical-diatomic molecule reactions to radical-polyatomic molecule reactions, members of the bimolecular gas-phase dynamics community have often used H-atom abstraction from methane (or one of its isotopologues) by X (where X=H, F or Cl) as a model system. Each of these model reactions can be separately characterized by both the height and location of the potential energy barrier along the reaction coordinate. Currently, we are working to understand the gas-phase dynamics of H-atom abstraction from CH_4 when X=Br. In this iteration of the model system, the abstraction barrier is located very late along the reaction coordinate and is quite high by comparison to other studied systems. This leads to some surprising dynamical effects in the X=Br system that we have not seen in other systems studied thus far.